

201-16624B

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# I U C L I D

## Data Set

**Existing Chemical** : ID: 88-85-7  
**CAS No.** : 88-85-7  
**EINECS Name** : dinoseb  
**EC No.** : 201-861-7  
**TSCA Name** : Phenol, 2-(1-methylpropyl)-4,6-dinitro-  
**Molecular Formula** : C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub>

**Producer related part**  
**Company** : Epona Associates, LLC  
**Creation date** : 28.11.2006

**Substance related part**  
**Company** : Epona Associates, LLC  
**Creation date** : 28.11.2006

**Status** :  
**Memo** : Chemtura DNBP

**Printing date** : 20.12.2006  
**Revision date** :  
**Date of last update** : 20.12.2006

**Number of pages** : 17

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10  
**Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4  
**Flags (profile)** : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),  
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1. General Information

Id 88-85-7

Date 20.12.2006

### 1.0.1 APPLICANT AND COMPANY INFORMATION

Type : cooperating company  
Name : Chemtura Corporation  
Contact person :  
Date :  
Street :  
Town :  
Country :  
Phone :  
Telefax :  
Telex :  
Cedex :  
Email :  
Homepage :

28.11.2006

### 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

### 1.0.3 IDENTITY OF RECIPIENTS

### 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

#### 1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance  
Substance type : organic  
Physical status : solid  
Purity : 98.5 % v/v  
Colour : yellow to brown  
Odour :

Remark : Purity of test substance was 98.5%  
28.11.2006

#### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

### 1.3 IMPURITIES

## **1. General Information**

**Id** 88-85-7

**Date** 20.12.2006

### **1.4 ADDITIVES**

### **1.5 TOTAL QUANTITY**

#### **1.6.1 LABELLING**

#### **1.6.2 CLASSIFICATION**

#### **1.6.3 PACKAGING**

### **1.7 USE PATTERN**

#### **1.7.1 DETAILED USE PATTERN**

#### **1.7.2 METHODS OF MANUFACTURE**

### **1.8 REGULATORY MEASURES**

#### **1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES**

#### **1.8.2 ACCEPTABLE RESIDUES LEVELS**

#### **1.8.3 WATER POLLUTION**

#### **1.8.4 MAJOR ACCIDENT HAZARDS**

#### **1.8.5 AIR POLLUTION**

#### **1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES**

#### **1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS**

#### **1.9.2 COMPONENTS**

## **1. General Information**

**Id** 88-85-7

**Date** 20.12.2006

**1.10 SOURCE OF EXPOSURE**

**1.11 ADDITIONAL REMARKS**

**1.12 LAST LITERATURE SEARCH**

**1.13 REVIEWS**

## 2. Physico-Chemical Data

Id 88-85-7

Date 20.12.2006

### 2.1 MELTING POINT

### 2.2 BOILING POINT

Value : 332 °C at  
Decomposition :  
Method : other  
Year :  
GLP : no data  
Test substance : as prescribed by 1.1 - 1.4

Remark : With the vapor pressure of 1.0 torr at 151.1 °C reported for this chemical in EXTOKNET, EPA calculated a boiling point of 340.5 °C using the NOMO5 program and a boiling point of 372 °C using the MPBPVP program in EPIWIN v.3.11.

Reliability : (2) valid with restrictions  
Another estimated boiling point of 362 °C was reported in a secondary source (Mackay et al. 2000). The boiling point of 332 °C is in good agreement with these calculated or estimated values.

Flag : Critical study for SIDS endpoint

20.12.2006

(4) (5)

### 2.3 DENSITY

#### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

### 2.5 PARTITION COEFFICIENT

#### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

#### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

## 2. Physico-Chemical Data

Id 88-85-7

Date 20.12.2006

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

### 3. Environmental Fate and Pathways

Id 88-85-7

Date 20.12.2006

#### 3.1.1 PHOTODEGRADATION

#### 3.1.2 STABILITY IN WATER

#### 3.1.3 STABILITY IN SOIL

#### 3.2.1 MONITORING DATA

#### 3.2.2 FIELD STUDIES

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

#### 3.3.2 DISTRIBUTION

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

#### 3.5 BIODEGRADATION

Type	: aerobic
Inoculum	: predominantly domestic sewage
Concentration	: 33.33 mg/l related to Test substance related to
Contact time	: 29 day(s)
Degradation	: 23.97 (±) % after 29 day(s)
Result	: other
Kinetic of testsubst.	: 9 day(s) 9.17 % % % % %
Control substance	: Acetic acid, sodium salt
Kinetic	: 29 day(s) 100 % %
Deg. product	: no
Method	: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year	: 2006
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Method	: The test item was tested at a concentration of 33.33 mg/L in mineral medium (= 16.67 mg TOC), along with inoculum controls, toxicity control and positive control. The CO2 released was measured on the 3rd, 6th, 9th, 14th, 19th, 24th and 29th day after initiation of the test.
Result	: The percent degradation of the the toxicity control was 45.09 at the end of the test.

### 3. Environmental Fate and Pathways

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Date 20.12.2006

Test substance : Based on the pass levels (60% in a 10-d window), the test  
Reliability : item was considered as non-biodegradable.  
Flag : Purity = 98.5%  
28.11.2006 : (1) valid without restriction  
: Critical study for SIDS endpoint

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#### 3.6 BOD5, COD OR BOD5/COD RATIO

#### 3.7 BIOACCUMULATION

#### 3.8 ADDITIONAL REMARKS



## 4. Ecotoxicity

Id 88-85-7

Date 20.12.2006

### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	: Scenedesmus subspicatus (Algae)
Endpoint	: growth rate
Exposure period	: 72 hour(s)
Unit	: mg/l
NOEC	: .03
LOEC	: .081 -
Limit test	: no
Analytical monitoring	: yes
Method	: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	: 2006
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Method	: The test item was tested at .030, .081, .219, .590 and 1.594 mg/L along with negative and positive controls. The cell growth was measured at 24, 48 and 72 hours after initiation of the test.
Result	: The 72 hour values were: EbC50 = .21 mg/L ErC50 = .74 mg/L NOEC = .030 mg/L LOEC = .081 mg/L
Test substance	: Purity = 98.5%
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint

28.11.2006

(1)

### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

#### 4.5.1 CHRONIC TOXICITY TO FISH

#### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

#### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

#### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

#### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

## 4. Ecotoxicity

Id 88-85-7

Date 20.12.2006

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

## 5. Toxicity

Id 88-85-7

Date 20.12.2006

### 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

#### 5.1.1 ACUTE ORAL TOXICITY

#### 5.1.2 ACUTE INHALATION TOXICITY

#### 5.1.3 ACUTE DERMAL TOXICITY

#### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

#### 5.2.1 SKIN IRRITATION

#### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

### 5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Cytogenetic assay
System of testing	: Chinese Hamster Ovary cells
Test concentration	: 75, 150 and 300 ug/ml (with activation); 55, 110 and 220 ug/ml (without activation)
Cytotoxic concentr.	: 300 ug/ml (with activation); 150 ug/ml (without activation)
Metabolic activation	: with and without
Result	: positive
Method	: OECD Guide-line 473
Year	: 2006
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Method	: One trial each, in the presence and absence of metabolic activation, was conducted. CHO cells were exposed to the test item in quadruplicate for 3 hours.
Result	: The respective positive control items produced a large and statistically significant increase in aberrant metaphases, under identical conditions.
Test substance	: Purity = 98.5%
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint
18.12.2006	

## 5. Toxicity

Id 88-85-7

Date 20.12.2006

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

**6.1 ANALYTICAL METHODS**

**6.2 DETECTION AND IDENTIFICATION**

**7.1 FUNCTION**

**7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED**

**7.3 ORGANISMS TO BE PROTECTED**

**7.4 USER**

**7.5 RESISTANCE**

**8.1 METHODS HANDLING AND STORING**

**8.2 FIRE GUIDANCE**

**8.3 EMERGENCY MEASURES**

**8.4 POSSIB. OF RENDERING SUBST. HARMLESS**

**8.5 WASTE MANAGEMENT**

**8.6 SIDE-EFFECTS DETECTION**

**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

**8.8 REACTIVITY TOWARDS CONTAINER MATERIAL**

## 9. References

Id 88-85-7

Date 20.12.2006

- (1) Advinus Therapeutics Private Limited (2006) Algal Growth Inhibition Test with 2-Sec Butyl-4,6 Dinitrophenol (CAS RN: 88-85-7)
- (2) Advinus Therapeutics Private Limited (2006) In vitro Chromosome Aberration Test with 2-Sec Butyl-4,6 Dinitrophenol (CAS RN: 88-85-7)
- (3) Advinus Therapeutics Private Limited (2006) Ready Biodegradability: CO2 Evolution Test with 2-Sec Butyl-4,6 Dinitrophenol (CAS RN: 88-85-7)
- (4) Extension Toxicology Network (EXTOXNET) (provided by US EPA)
- (5) Syracuse Research Corporation's PhysProp Database (provided by US EPA)



### 10.1 END POINT SUMMARY

### 10.2 HAZARD SUMMARY

### 10.3 RISK ASSESSMENT